Non-iterative and exact method for constraining particles in a linear geometry

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Abstract

We present a practical numerical method for evaluating the Lagrange multipliers necessary for maintaining a constrained linear geometry of particles in dynamical simulations. The method involves no iterations, and is limited in accuracy only by the numerical methods for solving small systems of linear equations. As a result of the non-iterative and exact (within numerical accuracy) nature of the procedure there is no drift in the constrained geometry, and the method is therefore readily applied to molecular dynamics simulations of, e.g., rigid linear molecules or materials of non-spherical grains. We illustrate the approach through implementation in the commonly used second-order velocity explicit Verlet method.

I. INTRODUCTION

Computational studies of the dynamics and statistics of large particle ensembles have been successfully conducted for several decades [1,2], and many different types of inter-particle force fields have been developed for specific physical applications. The particles of interest in Molecular Dynamics (MD) or Discrete Element Methods (DEMs) are often represented by spatial point coordinates and the associated momenta. For example, atomic-scale modeling of materials considers each atom as a point particle, and the nature of the material is defined by the interatomic potential. Likewise, the dynamics of inhomogeneous atomic ensembles, such as molecular chains in solution, can be modeled by point particles with different interaction potentials defining the nature of the chemistry between two or more atoms. Given a complex ensemble of interactions, the involved time scales of the dynamics may span many orders of magnitude, thereby limiting the efficiency of a simulation approach since a useful numerical time step for a simulation is inversely proportional to the highest frequency in the system. Thus, if particles interact such that high-frequency, small-amplitude oscillations result, it may be advantageous to disregard the dynamics of the interaction and constrain the relative degree of freedom between the two objects to the mean distance. In molecular systems at room temperature conditions, constraints are further justified by the fact that many relevant chemical bond vibrations are improbable to be found in an excited quantum mechanical energy state. Other examples of the application of holonomic constraints can be found in studies of granular materials composed of non-spherical particles. Many such studies relate to particles of complex geometry or to particles that are connected through actual physical constraints. Modeling these systems by spherical particles interacting through vibrational potentials is obviously not desirable as it may introduce spurious deformations and internal oscillations.

As a result of the interest in constraints, much work has been devoted in the literature to develop practical, accurate, and efficient methods for introducing constraints into the numerical methods to study the dynamics of non-spherical particles. Much of the pioneering work culminated in the SHAKE [3] and RATTLE [4] algorithms. These methods consider the constraints in a (point) particle ensemble as a collection of linearly independent constraints on distances between pairs of particles. For any given time step of a numerical temporal integrator of the equations of motion for each particle, the constraints are enforced for the resulting positions through the self-consistent solution of a set of nonlinear equations (one for each constraint). This solution is usually obtained through an iterative approach where computational efficiency has to be balanced with the desire for accuracy. These approaches have been very successful and are still the core in many applications. Some modifications have been introduced for specific systems and geometries. For example, SETTLE [5] provides a direct analytical calculation of the three constraints necessary for rigid triangular objects (developed for three-point classical water models), and "Fast SHAKE" [6] optimizes the iterative method for finding the constraints necessary for modeling small rigid molecules. Other suggestions include the EEM approach [7,8], which evaluates the constraints non-iteratively at the beginning of a time step where all positions are known. As a consequence of iterative methods and algorithmic approximations, the updated positions do not exactly fulfill the holonomic constraints, and corrective measures must be applied if and when the cumulative discrepancy becomes unacceptable.

Most methods for evaluating constraints have been developed for ensembles of linearly independent constraints. Several publications, including [3], consider the linear geometry as a separate case due to occurring singularities in the methods for linearly independent constraints. A few direct methods for linear geometry have been outlined (see, e.g., [9]), but they are possible only because of perfect three-body symmetry. We demonstrate a simple method for evaluating the necessary Lagrange multipliers for constraining any number of different particles onto a *linear* geometry. We show that the resulting method is efficient, non-iterative, exact, and self-correcting.

II. EQUATIONS OF MOTION WITH CONSTRAINTS

We consider the dynamics of N particles constrained on a straight line (see Figure 1). The equations of motion for the coordinate, $\bar{R}_j$, of the jth particle is given by:

$$m_j \ddot{\bar{R}}_j + \alpha_j \dot{\bar{R}}_j = \bar{\mathcal{F}}_j = \begin{cases} \bar{f}_1 + \lambda_{1N} \bar{R}_{1N} - l_{1N} \sum\limits_{k=2}^{N-1} \bar{\lambda}_{k1} & , \quad j = 1 \\ \bar{f}_j + l_{1N}(\bar{\lambda}_{j1} + \bar{\lambda}_{jN}) & , \ 1 < j < N \quad , \\ \bar{f}_N - \lambda_{1N} \bar{R}_{1N} - l_{1N} \sum\limits_{k=2}^{N-1} \bar{\lambda}_{kN} & , \quad j = N \end{cases} \tag{1}$$

where m_j is the mass, friction is represented by α_j, and $\bar{f}_j$ is an extra-molecular force on the jth particle. Throughout the paper, overbar "$\rightarrow$" and overdot "·" denote a vector and a temporal derivative, respectively. The two particles, $j = 1$ and $j = N$, define the direction and length of the object through the scalar Lagrange multiplier λ_{1N} and the vector $\bar{R}_{1N} = \bar{R}_N - \bar{R}_1$. The length l_{ji} is defined by $l_{ji} = |\bar{R}_i - \bar{R}_j|$. All other particles, $1 < j < N$, are constrained to their relative positions through the vector multipliers $\bar{\lambda}_{ji}$ for $i = 1, N$, that connect each of those particles exclusively to the defining particles of $j = 1, N$. Notice that all the forces of the constraints cancel for the ensemble. At any given time the constraints are enforced by the geometric conditions:

$$\left| \bar{R}_{1N} \right| = l_{1N} \tag{2}$$

$$\bar{R}_j = \frac{l_{jN} \bar{R}_1 + l_{j1} \bar{R}_N}{l_{1N}} \ , \tag{3}$$

where all particles $1 < j < N$ lie between particles 1 and N, such that $l_{j1} + l_{jN} = l_{1N}$. The number of geometrical conditions given in (2) and (3) is $3(N-2) + 1$ (three-dimensional space), whereas the number of Lagrange multipliers to be determined for the solution of (1) is $6(N-2) + 1$. Since the constraints should not contribute net torque to the object, we further have the conditions for $1 < j < N$:

$$\bar{R}_{1N} \times \left(l_{j1} \bar{\lambda}_{j1} - l_{jN} \bar{\lambda}_{jN} \right) = 0 \ . \tag{4}$$

By writing

$$\bar{\lambda}_{ji} = \bar{\lambda}_{ji}^{\parallel} + \bar{\lambda}_{ji}^{\perp} \ , \tag{5}$$

with $\bar{\lambda}_{ji}^{\perp} \cdot \bar{R}_{1N} = 0$ and $\bar{\lambda}_{ji}^{\parallel} = \lambda_{ji}^{\parallel} \bar{R}_{1N}/|\bar{R}_{1N}|$, we can express (4) in the form

$$l_{j1}\bar{\lambda}_{j1}^{\perp} = l_{jN}\bar{\lambda}_{jN}^{\perp} \ , \tag{6}$$

i.e., the constraint forces, responsible for maintaining particle j at its desired relative position, are balanced in their components orthogonal to the direction of the object such that no net torque is contributed.

However, it is important to realize that this balance does not necessarily apply to the longitudinal components, $\lambda_{j1}^{\parallel}$ and $\lambda_{jN}^{\parallel}$. Since the object is rigid, we may therefore choose *any* number, γ_j $(1 < j < N)$, such that

$$\gamma_j \bar{\lambda}_{j1}^{\parallel} = \bar{\lambda}_{jN}^{\parallel} \tag{7}$$

without any physical consequence. This ambiguity reflects the physical fact that a rigid stick responds identically regardless of how *longitudinal* forces are distributed along the object. Inserting (6) and (7) into (1), we can thereby obtain the following system of equations

$$m_j\ddot{\bar{R}}_j + \alpha_j\dot{\bar{R}}_j = \begin{cases} \bar{f}_1 + \lambda_{1N}\bar{R}_{1N} - l_{1N}\sum_{k=2}^{N-1}\left(\bar{\lambda}_{k1}^{\perp} + \bar{\lambda}_{k1}^{\parallel}\right) & , \quad j = 1 \\ \bar{f}_j + l_{1N}\frac{l_{1N}}{l_{j1}}\bar{\lambda}_{j1}^{\perp} + l_{1N}(1+\gamma_j)\bar{\lambda}_{j1}^{\parallel} & , \quad 1 < j < N \quad , \\ \bar{f}_N - \lambda_{1N}\bar{R}_{1N} - l_{1N}\sum_{k=2}^{N-1}\left(\frac{l_{kN}}{l_{k1}}\bar{\lambda}_{k1}^{\perp} + \gamma_k\bar{\lambda}_{k1}^{\parallel}\right) & , \quad j = N \end{cases} \tag{8}$$

with $3(N-2)+1$ Lagrange multipliers, determined by the geometry of (2) and (3) (notice that the vector $\bar{\lambda}_{k1} = \bar{\lambda}_{k1}^{\perp} + \bar{\lambda}_{k1}^{\parallel}$ represents 3 scalar multipliers, one for the longitudinal direction $\bar{\lambda}_{k1}^{\parallel}$ and two for orthogonal directions $\bar{\lambda}_{k1}^{\perp}$). These equations can now be introduced into a variety of numerical integrators, determining the Lagrange multipliers for enforcing the constraints, and exploiting the free Gauge parameters, γ_j, for computational optimization.

III. USING THE VELOCITY EXPLICIT VERLET METHOD

In the following we illustrate the approach through the commonly used [2,4] velocity Explicit Verlet algorithm (shown here including linear damping) which approximates the solution to (1) using a non-zero time step of dt connecting time $t_n = ndt$ to $t_{n+1} = (n+1)dt$,

$$\bar{R}_j^{n+1} = \bar{R}_j^n + \left(1 - \frac{\alpha_j dt}{2}\right)dt\bar{V}_j^n + \frac{dt^2}{2m_j}\bar{\mathcal{F}}_j^n \tag{9}$$

$$\bar{V}_j^{n+1} = \frac{1 - \frac{\alpha_j dt}{2}}{1 + \frac{\alpha_j dt}{2}}\bar{V}_j^n + \frac{1}{1 + \frac{\alpha_j dt}{2}}\frac{dt}{2m_j}\left(\bar{\mathcal{F}}_j^n + \bar{\mathcal{F}}_j^{n+1}\right) \ , \tag{10}$$

where we use the notation, $\bar{X}_j^n = \bar{X}_j(t_n) = \bar{X}_j(n \cdot dt)$, to describe the integer n time step, and where $\bar{V}_j = \dot{\bar{R}}_j$.

A. Determining the Lagrange Multipliers $\bar{\lambda}_{ji}$

Inserting (8) into (9) yields the constrained discrete-time equations

$$\bar{R}_j^{n+1} = \tilde{R}_j^{n+1} + \mathcal{A}_j \times \begin{cases} \lambda_{1N}\bar{R}_{1N}^n - l_{1N}\displaystyle\sum_{k=2}^{N-1}\left(\bar{\lambda}_{k1}^\perp + \bar{\lambda}_{k1}^\parallel\right) , & j = 1 \\[2mm] l_{1N}\dfrac{l_{1N}}{l_{j1}}\bar{\lambda}_{j1}^\perp + l_{1N}(1+\gamma_j)\bar{\lambda}_{j1}^\parallel , & 1 < j < N \\[2mm] -\lambda_{1N}\bar{R}_{1N}^n - l_{1N}\displaystyle\sum_{k=2}^{N-1}\left(\dfrac{l_{kN}}{l_{k1}}\bar{\lambda}_{k1}^\perp + \gamma_k\bar{\lambda}_{k1}^\parallel\right) , & j = N \end{cases} \tag{11}$$

with $\mathcal{A}_j = \frac{dt^2}{2m_j}$ and, following the notation of [2,4], $\tilde{R}_j^{n+1}$ is the updated (vector) position of particle j, had there been no constraints. The longitudinal and orthogonal components of $\bar{\lambda}_{ji}$ are here relative to $\bar{R}_{1N}^n$. The Lagrange multipliers are now determined such that the constraints are satisfied at time t_{n+1}; i.e., under the conditions

$$\left|\bar{R}_{1N}^{n+1}\right|^2 = l_{1N}^2 \tag{12}$$

$$1 < j < N: \quad \bar{R}_j^{n+1} = \frac{l_{jN}\bar{R}_1^{n+1} + l_{j1}\bar{R}_N^{n+1}}{l_{1N}} . \tag{13}$$

Inserting (11) into (12) provides us with one equation for the determination of λ_{1N},

$$l_{1N}^2 = \Big|\overbrace{\tilde{R}_{1N}^{n+1} + l_{1N}\sum_{k=2}^{N-1}\left(\mathcal{A}_1 - \mathcal{A}_2\frac{l_{k1}}{l_{k2}}\right)\bar{\lambda}_{k1}^\perp}^{\bar{\rho}} + l_{1N}\underbrace{\sum_{k=2}^{N-1}(\mathcal{A}_1 - \mathcal{A}_N\gamma_k)\,\bar{\lambda}_{k1}^\parallel}_{=0\ \text{for}\ \gamma_k=\mathcal{A}_1/\mathcal{A}_N} - (\mathcal{A}_1 + \mathcal{A}_N)\bar{R}_{1N}^n\lambda_{1N}\Big|^2 ,$$

$$\tag{14}$$

whereas inserting (11) into (13) provides us with $3(N-2)$ equations for the determination of $\bar{\lambda}_{j1}$,

$$-\mathcal{A}_j\frac{l_{1N}^2}{l_{jN}}\bar{\lambda}_{j1}^\perp - \sum_{k=2}^{N-1}\left(l_{jN}\mathcal{A}_1 + l_{j1}\frac{l_{k1}}{l_{kN}}\mathcal{A}_N\right)\bar{\lambda}_{k1}^\perp = \Delta\tilde{R}_j^\perp \tag{15}$$

$$-\mathcal{A}_j l_{1N}(1+\gamma_j)\bar{\lambda}_{j1}^\parallel - \sum_{k=2}^{N-1}(l_{1N}\mathcal{A}_1 - \underbrace{l_{j1}\left(\mathcal{A}_1 - \gamma_k\mathcal{A}_N\right)}_{=0\ \text{for}\ \gamma_k=\mathcal{A}_1/\mathcal{A}_N})\bar{\lambda}_{k1}^\parallel = \Delta\tilde{R}_j^\parallel - \frac{\bar{R}_{1N}^n}{l_{1N}}\left(\mathcal{A}_1 l_{jN} - \mathcal{A}_N l_{j1}\right)\lambda_{1N} ,$$

$$\tag{16}$$

where

$$\Delta\tilde{R}_j = \Delta\tilde{R}_j^\perp + \Delta\tilde{R}_j^\parallel\frac{\bar{R}_{1N}^n}{\left|\bar{R}_{1N}^n\right|} = \tilde{R}_j^{n+1} - \frac{l_{jN}\tilde{R}_1^{n+1} + l_{j1}\tilde{R}_N^{n+1}}{l_{1N}} . \tag{17}$$

Solving equations (14)-(16) will provide the Lagrange multipliers. However, since (14) is a nonlinear equation, and since (14)-(16) are coupled, the direct solution to the equations will require an iterative approach to the solution of the $3(N-2)+1$ equations. A significant

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computational consequence of separating the orthogonal and longitudinal components of the Lagrange multiplier $\bar{\lambda}_{j1}$ is that the "free" parameters γ_j (for $1 < j < N$) introduced in (7) can now be chosen to optimize efficiency. Specifically, choosing $\gamma_j = \mathcal{A}_1/\mathcal{A}_N = m_N/m_1$ leads to the following *efficient, non-iterative, exact,* and *self-correcting* procedure for evaluating the necessary multipliers:

Step 1: Solve the two independent sets of $N - 2$ linear equations (15) to obtain $\bar{\lambda}_{j1}^{\perp}$.

Step 2: Solve (14). With $\bar{\lambda}_{j1}^{\perp}$ evaluated, then $\bar{\rho}$ is known. Given $\gamma_j = \mathcal{A}_1/\mathcal{A}_N$, this equation becomes a simple second-order polynomial in λ_{1N} where the root closer to zero is the relevant one.

Step 3: With the completion of steps 1 and 2, $\lambda_{j1}^{\parallel}$ can be found from (16) (with $\gamma_j = \mathcal{A}_1/\mathcal{A}_N$) as the solution to the set of $N - 2$ linear equations.

The facts that the method outlined above is non-iterative and exact are self-evident. Given that the involved matrices are rather small ($(N - 2) \times (N - 2)$), the method is also computationally efficient. Finally, it can be seen that regardless of deviations from the desired constrained geometry at time $n \cdot dt$, the geometric conditions for evaluating the Lagrange multipliers are enforced at time $(n + 1) \cdot dt$ (see (12) and (13)). Thus, the method is self-correcting when making the important distinction between, e.g., a *desired* length l_{j1} and an *actual* length $|\bar{R}_{j1}^n|$, which may not be equal to l_{j1} due to computational precision errors.

The matrices corresponding to the $N - 2$ equations in (15) and (16) are generally very well conditioned and are not subject to numerical instabilities. Specifically, for a system of N equal masses the matrix described in (16) has condition number [10] $k_2^{\parallel} = \frac{1}{2}N$ (for $N > 3$). The matrix (15) describing the orthogonal components of the Lagrange multipliers is less transparent. However, for a system of evenly spaced equal masses, we show in Figure 2 how the condition number $k_2^{\perp}$ depends on N. It is clear from these data that the matrices are easily handled numerically for any reasonable number of constrained particles. It is important to realize that the matrix (15) may become less well conditioned if $\mathcal{A}_N/l_{jN}$ is extremely large for any $0 < j < N$. However, (11) and (15) have been expressed in terms of $\bar{\lambda}_{j1}$, through the relationships (6) and (7). Thus, we could equally well have chosen the sought after Lagrange multipliers to be $\bar{\lambda}_{jN}$, in which case equations equivalent to (15)-(17) can be produced to avoid a possible ill conditioned matrix for large $\mathcal{A}_N/l_{jN}$. It is also important to realize that these matrices are not changing during the course of a simulation, and that, e.g., the same *LU* factorization can be effectively used for all time steps. The solution to (14) is limited mainly by $\bar{\rho}$, as it can be seen that the polynomial may have only complex solutions when $\bar{\rho}$ is near orthogonal to $\bar{R}_{1N}^n$. For reasonable time steps, when particle positions only change by a fraction of particle size, $\bar{\rho}$ is always near parallel to $\bar{R}_{1N}^n$, and (14) does therefore not pose any unpredictable numerical problems.

The completion of the time step in (11) can then be accomplished for all participating particles in an ensemble. With these new coordinates at time t_{n+1}, the resulting forces $\bar{f}_j^{n+1}$ can be evaluated.

B. Updating the Velocities

As pointed out in [4], straightforward application of (10) will not in general satisfy the necessary constraints on the velocity complements to (12) and (13):

$$\bar{V}_{1N}^{n+1} \cdot \bar{R}_{1N}^{n+1} = 0 \tag{18}$$

$$1 < j < N: \quad \bar{V}_j^{n+1} = \frac{l_{jN}\bar{V}_1^{n+1} + l_{j1}\bar{V}_N^{n+1}}{l_{1N}}. \tag{19}$$

The necessary corrections can be introduced by the following modification,

$$\bar{\mathcal{F}}_j^{n+1} = \bar{f}_j^{n+1} + \mathcal{B}_j \times \begin{cases} \sigma_{1N}\bar{R}_{1N}^{n+1} - l_{1N}\sum_{k=2}^{N-1}\bar{\sigma}_{k1}, & j = 1 \\ l_{1N}(\bar{\sigma}_{j1} + \bar{\sigma}_{jN}), & 1 < j < N \\ -\sigma_{1N}\bar{R}_{1N}^{n+1} - l_{1N}\sum_{k=2}^{N-1}\bar{\sigma}_{k1}, & j = N \end{cases} \tag{20}$$

where $\mathcal{B}_j = dt/(2m_j + \alpha_j dt)$. As for the Lagrange multipliers $\bar{\lambda}_{ji}$ the introduction of $\bar{\sigma}_{ji}$ should conserve angular momentum, i.e.,

$$l_{j1}\bar{\sigma}_{j1}^{\perp} = l_{jN}\bar{\sigma}_{jN}^{\perp} \tag{21}$$

$$\delta_j\bar{\sigma}_{j1}^{\parallel} = \bar{\sigma}_{jN}^{\parallel}, \tag{22}$$

where $\bar{\sigma}_{ji} = \bar{\sigma}_{ji}^{\perp} + \bar{\sigma}_{ji}^{\parallel}$ with $\bar{\sigma}_{ji}^{\perp} \cdot \bar{R}_{1N}^{n+1} = 0$ and $\bar{\sigma}_{ji}^{\parallel} \| \bar{R}_{1N}^{n+1}$. Analogous to the physically arbitrary coefficient γ_j, here we have coefficients δ_j that can be chosen to be any number. With this observation, (20) becomes the velocity complement to (11):

$$\bar{V}_j^{n+1} = \tilde{V}_j^{n+1} + \mathcal{B}_j \times \begin{cases} \sigma_{1N}\bar{R}_{1N}^{n+1} - l_{1N}\sum_{k=2}^{N-1}\left(\bar{\sigma}_{k1}^{\perp} + \bar{\sigma}_{k1}^{\parallel}\right), & j = 1 \\ l_{1N}\frac{l_{1N}}{l_{j1}}\bar{\sigma}_{j1}^{\perp} + l_{1N}(1 + \delta_j)\bar{\sigma}_{j1}^{\parallel}, & 1 < j < N \\ -\sigma_{1N}\bar{R}_{1N}^{n+1} - l_{1N}\sum_{k=2}^{N-1}\left(\frac{l_{kN}}{l_{k1}}\bar{\sigma}_{k1}^{\perp} + \delta_k\bar{\sigma}_{k1}^{\parallel}\right), & j = N \end{cases} \tag{23}$$

The (vector) velocities without the corrective multipliers $\bar{\sigma}$ are denoted $\tilde{V}_j^{n+1}$. The velocity equations are now determined by inserting (23) into (18) and (19), yielding the following set of $3(N-2) + 1$ linear equations,

$$\Delta\tilde{V}_j^{\perp} = -\mathcal{B}_j\frac{l_{1N}^2}{l_{jN}}\bar{\sigma}_{j1}^{\perp} - \sum_{k=2}^{N-1}\left(l_{jN}\mathcal{B}_1 + l_{j1}\frac{l_{k1}}{l_{kN}}\mathcal{B}_N\right)\bar{\sigma}_{k1}^{\perp} \tag{24}$$

$$\sigma_{1N} = \frac{\bar{R}_{1N}^{n+1} \cdot \tilde{V}_{1N}^{n+1} + l_{1N}\overbrace{\sum_{k=2}^{N-1}(\mathcal{B}_1 - \delta_k\mathcal{B}_N)\bar{\sigma}_{k1}}^{=0 \text{ for } \delta_k = \mathcal{B}_1/\mathcal{B}_N}}{\left|\bar{R}_{1N}^{n+1}\right|^2(\mathcal{B}_1 + \mathcal{B}_N)} \tag{25}$$

$$\Delta\tilde{V}_j^{\parallel} - \frac{\bar{R}_{1N}^{n+1}}{l_{1N}}(\mathcal{B}_1 l_{jN} - \mathcal{B}_N l_{j1})\sigma_{1N} = -\mathcal{B}_j l_{1N}(1 + \delta_j)\bar{\sigma}_{j1}^{\parallel} - \sum_{k=2}^{N-1}(l_{1N}\mathcal{B}_1 - \underbrace{l_{j1}(\mathcal{B}_1 - \delta_k\mathcal{B}_N)}_{=0 \text{ for } \delta_k = \mathcal{B}_1/\mathcal{B}_N})\bar{\sigma}_{k1}^{\parallel}, \tag{26}$$

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where

$$\Delta \tilde{V}_j = \Delta \tilde{V}_j^{\perp} + \Delta \tilde{V}_j^{\parallel} \frac{\bar{R}_{1N}^{n+1}}{\left| \bar{R}_{1N}^{n+1} \right|} = \Delta \tilde{V}_j^{n+1} - \frac{l_{jN} \Delta \tilde{V}_1^{n+1} + l_{j1} \Delta \tilde{V}_N^{n+1}}{l_{1N}} . \tag{27}$$

The solution to the set of linear equations (24)-(26) can be significantly assisted by choosing $\delta_k = \mathcal{B}_1/\mathcal{B}_N$. This choice will allow (25) to become independent of the other equations, and all corrective multipliers σ can be obtained by solving three sets of $N-2$ (plus one) linear equations in the listed order. With this solution, the velocities $\bar{V}_j^{n+1}$ can be completed through (23), and the time step is then accomplished. Before initiating another time step, it is important to include the corrective multipliers into the evaluated force, i.e., $\bar{f}_j^{n+1} = \bar{\mathcal{F}}_j^{n+1}$, before evaluating $\tilde{R}_j^{n+2}$.

Notice that for small dt, the matrices given by (24) and (26) are nearly identical to the ones described by (15) and (16), respectively. Thus, we can assume that (24) and (26) are subject to very similar conditioning as discussed in the previous section, when solving the systems numerically.

IV. CONCLUSION

We have presented an efficient algorithm for conducting dynamical simulations of particles constrained in a linear geometry. Following other presentations on geometrical constraints in particle simulations, we introduce Lagrange multipliers to the equations of motion for each particle, and determine the multipliers by the desired constraints as well as basic conditions of conservation of momentum and angular momentum. The resulting equations for determining the Lagrange multipliers are, in general, a set of coupled equations with some nonlinear component, necessitating an iterative approach to obtain an approximate solution. By taking advantage of the physical ambiguity left in the distribution of the constraining forces in the longitudinal direction of the ensemble, we are able to determine a particular distribution that decouples the nonlinearity of the determining equations into a second-order polynomial of a single variable, namely, one of the Lagrange multipliers in the longitudinal direction. The rest of the equations are linear and can be solved as three independent sets of $N-2$ equations with $N-2$ unknowns, where N is the number of mutually constrained particles. Thus, the algorithm is exact (within the accuracy of floating-point arithmetic), efficient, and non-iterative. We have illustrated the approach through an implementation with the widely used velocity explicit Verlet algorithm for temporal integration of second-order differential equations. The presented formulation of the approach has the added benefit of being self-correcting, i.e., any spurious deviations in the constrained geometry arising from, e.g., computational precision error, is self-corrected, and the algorithm does not accumulate or propagate error in the constraints. It is straightforward to apply the method to other numerical methods for ordinary differential equations. For example, a recent comprehensive study on self-assembled monolayers [11] applied the above-outlined technique to model rigid and linear alkanethiol molecules as overdamped stochastically driven objects.

V. ACKNOWLEDGMENTS

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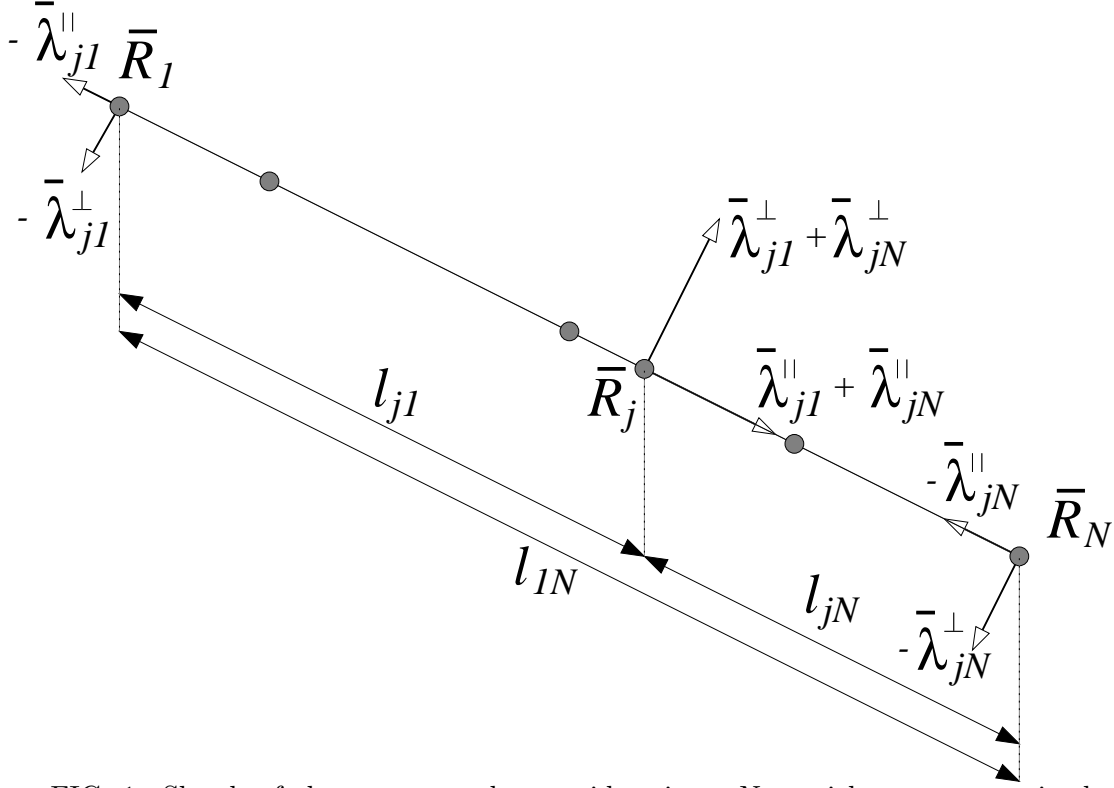
FIG. 1. Sketch of the system under consideration. N particles are constrained to the line, defined by $\bar{R}_N - \bar{R}_1$, through the Lagrange multipliers $\bar{\lambda}_{ji} = \bar{\lambda}_{ji}^{\perp} + \bar{\lambda}_{ji}^{\parallel}$, where $1 < j < N$ and $i = 1, N$.
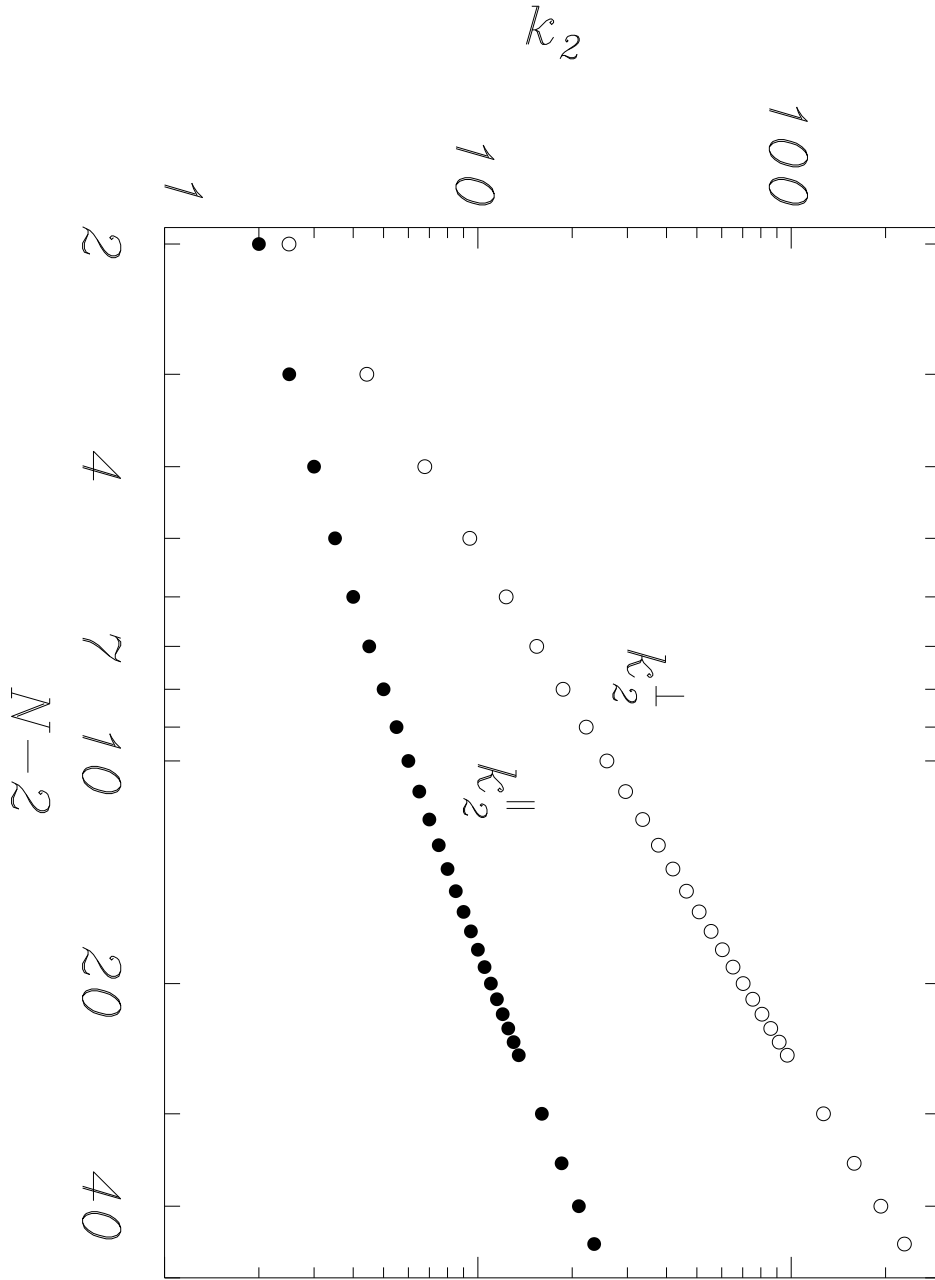
FIG. 2. Condition numbers, $k_2^{\perp}$ and $k_2^{\parallel}$, for the matrices described by equation (15) (∘) and equation (16) (•) for $\gamma_k = \mathcal{A}_1/\mathcal{A}_N$ as a function of the matrix size $(N-2) \times (N-2)$, if the N particles have equal mass and are evenly spaced along $\bar{R}_{1N}$. The condition numbers are $k_2^{\parallel} = \frac{1}{2}N$ and $k_2^{\perp} \approx (N-2)^{1.4}$.